



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:12 AM GMT

PDB ID : 3CXC
Title : The structure of an enhanced oxazolidinone inhibitor bound to the 50S ribosomal subunit of *H. marismortui*
Authors : Ippolito, J.A.; Wang, D.; Kanyo, Z.F.; Duffy, E.M.
Deposited on : 2008-04-24
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

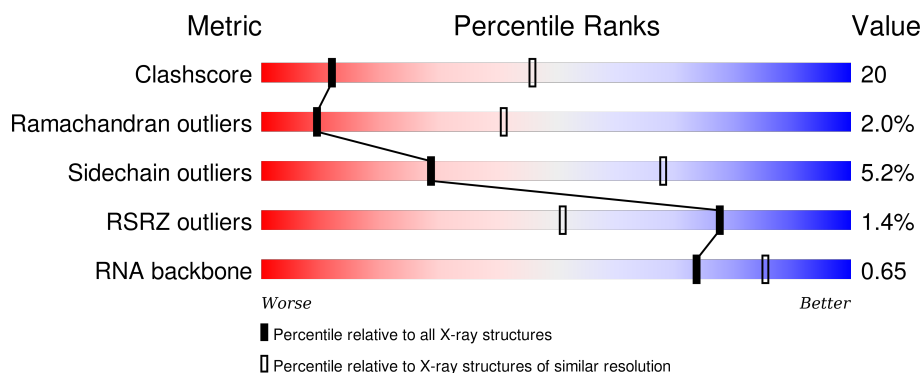
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>40%</div> <div>6%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>49%</div> <div>11%</div> <div>•</div> </div> </div>
3	4	3	<div> <div> <div></div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
4	A	239	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> <div>•</div> </div> </div>
5	B	337	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
6	C	246	
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	
15	L	194	
16	M	186	
17	N	115	
18	O	148	
19	P	95	
20	Q	154	
21	R	84	
22	S	119	
23	T	66	
24	U	70	
25	V	154	
26	W	91	
27	X	240	
28	Y	73	
29	Z	56	
30	1	48	

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Mol	Chain	Length	Quality of chain
31	2	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8006	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8049	-	-	-	X
33	MG	0	8053	-	-	-	X
33	MG	0	8054	-	-	-	X
33	MG	0	8064	-	-	-	X
33	MG	0	8108	-	-	-	X
34	K	0	8202	-	-	-	X
35	NA	0	8303	-	-	-	X
35	NA	0	8308	-	-	-	X
35	NA	0	8310	-	-	-	X
35	NA	0	8320	-	-	-	X
35	NA	0	8321	-	-	-	X
35	NA	0	8323	-	-	-	X
35	NA	0	8324	-	-	-	X
35	NA	0	8325	-	-	-	X
35	NA	0	8326	-	-	-	X
35	NA	0	8332	-	-	-	X
35	NA	0	8333	-	-	-	X
35	NA	0	8335	-	-	-	X
35	NA	0	8350	-	-	-	X
35	NA	0	8356	-	-	-	X
35	NA	0	8361	-	-	-	X
35	NA	0	8362	-	-	-	X
35	NA	0	8364	-	-	-	X
35	NA	0	8365	-	-	-	X
35	NA	0	8366	-	-	-	X
35	NA	0	8367	-	-	-	X
35	NA	0	8368	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8372	-	-	-	X
35	NA	0	8373	-	-	-	X
35	NA	0	8376	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8377	-	-	-	X
35	NA	0	8378	-	-	-	X
35	NA	0	8379	-	-	-	X
35	NA	9	8383	-	-	-	X
35	NA	K	8380	-	-	-	X
35	NA	Q	8386	-	-	-	X
36	CL	0	8505	-	-	-	X
36	CL	2	8504	-	-	-	X
36	CL	B	8519	-	-	-	X
36	CL	I	8521	-	-	-	X
36	CL	J	8512	-	-	-	X
37	CD	2	8404	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98635 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PRO	CONFLICT	UNP P20279

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	I	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	145	Total	C	N	O	S	0	0	0
			1118	670	222	226				

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	N	115	Total	C	N	O	S	0	0	0
			865	529	161	175				

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	O	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	P	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Q	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	R	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	S	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	T	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	U	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	V	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	W	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Z	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

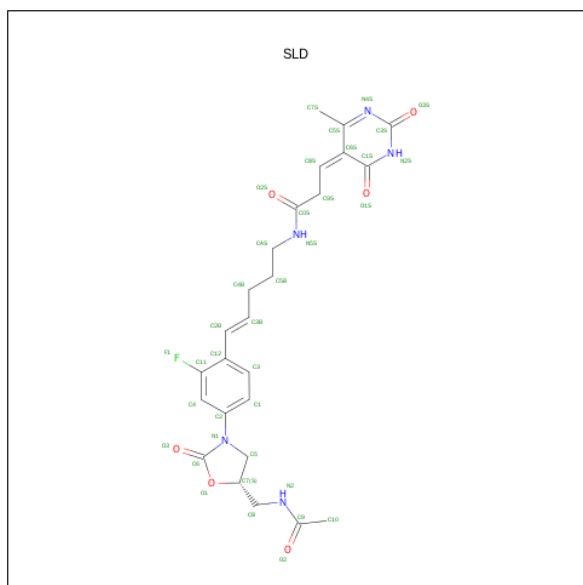
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	DELETION	UNP P22452

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is (3Z)-N-[(4E)-5-(4-{(5S)-5-[(ACETYLAMINO)METHYL]-2-OXO-1,3-OXAZOLIDIN-3-YL}-2-FLUOROPHENYL)PENT-4-EN-1-YL]-3-(4-METHYL-2,6-DIOXO-1,6-DIHYDROPYRIMIDIN-5(2H)-YLIDENE)PROPANAMIDE (three-letter code: SLD) (formula: C₂₅H₂₈FN₅O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	F	N	O	0	0
			37	25	1	5	6		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	J	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	2	1	Total 1	Mg 1	0	0
33	9	2	Total 2	Mg 2	0	0
33	S	1	Total 1	Mg 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total 2	K 2	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	73	Total 73	Na 73	0	0
35	P	1	Total 1	Na 1	0	0
35	Q	2	Total 2	Na 2	0	0
35	K	1	Total 1	Na 1	0	0
35	H	2	Total 2	Na 2	0	0
35	I	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	A	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	8	Total Cl 8 8	0	0
36	P	1	Total Cl 1 1	0	0
36	J	1	Total Cl 1 1	0	0
36	Q	1	Total Cl 1 1	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	X	1	Total Cl 1 1	0	0
36	2	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	Z	1	Total Cd 1 1	0	0
37	Y	1	Total Cd 1 1	0	0
37	T	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	N	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5806	Total 5806	O 5806	0	0
38	9	147	Total 147	O 147	0	0
38	4	1	Total 1	O 1	0	0
38	A	136	Total 136	O 136	0	0
38	B	160	Total 160	O 160	0	0
38	C	180	Total 180	O 180	0	0
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	26	Total 26	O 26	0	0
38	G	21	Total 21	O 21	0	0
38	H	82	Total 82	O 82	0	0
38	I	61	Total 61	O 61	0	0
38	J	63	Total 63	O 63	0	0
38	K	85	Total 85	O 85	0	0
38	L	130	Total 130	O 130	0	0
38	M	69	Total 69	O 69	0	0
38	N	45	Total 45	O 45	0	0
38	O	70	Total 70	O 70	0	0
38	P	56	Total 56	O 56	0	0
38	Q	92	Total 92	O 92	0	0
38	R	40	Total 40	O 40	0	0
38	S	37	Total 37	O 37	0	0

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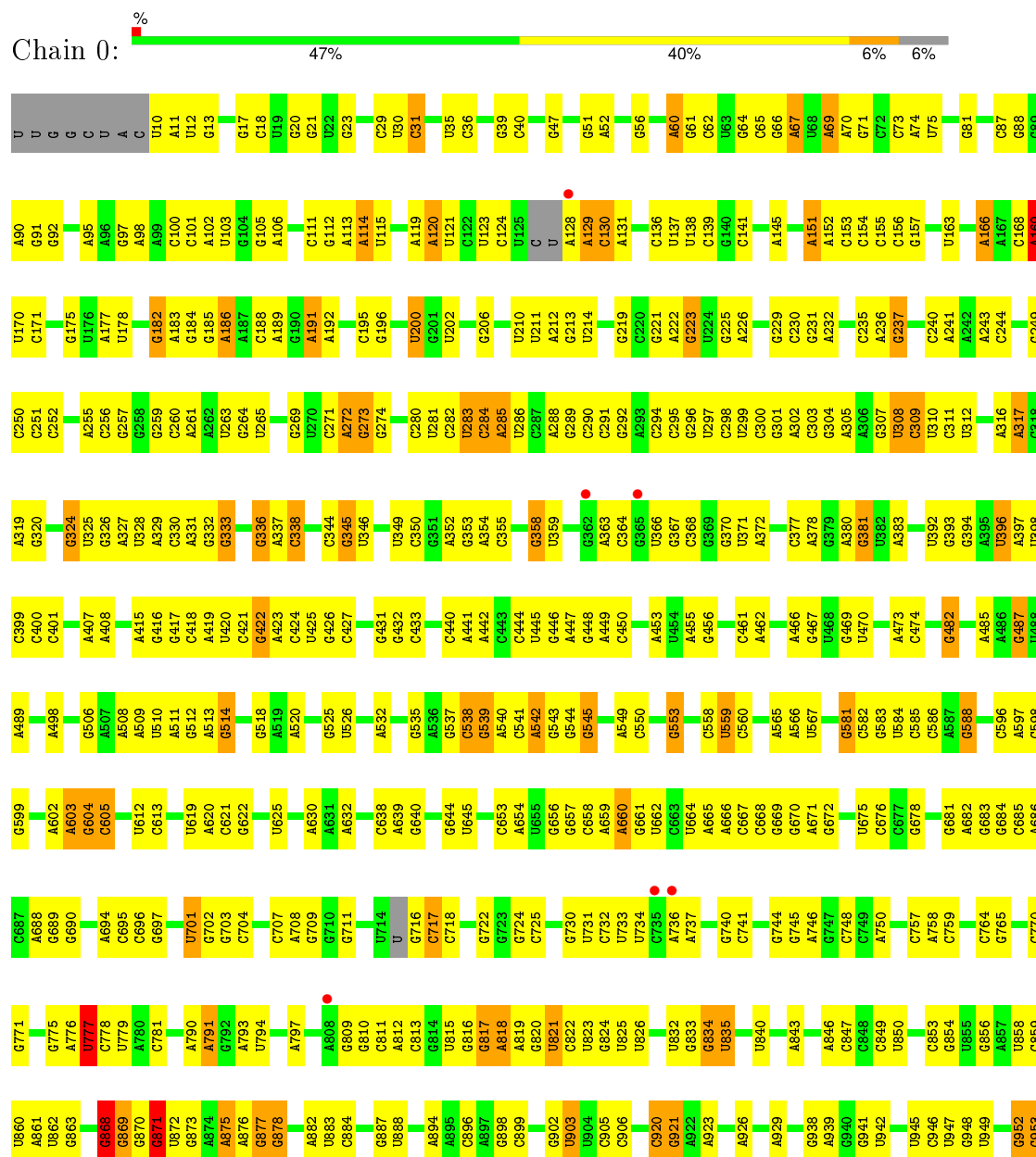
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	27	Total 27	O 27	0	0
38	U	13	Total 13	O 13	0	0
38	V	74	Total 74	O 74	0	0
38	W	29	Total 29	O 29	0	0
38	X	105	Total 105	O 105	0	0
38	Y	41	Total 41	O 41	0	0
38	Z	57	Total 57	O 57	0	0
38	1	45	Total 45	O 45	0	0
38	2	76	Total 76	O 76	0	0

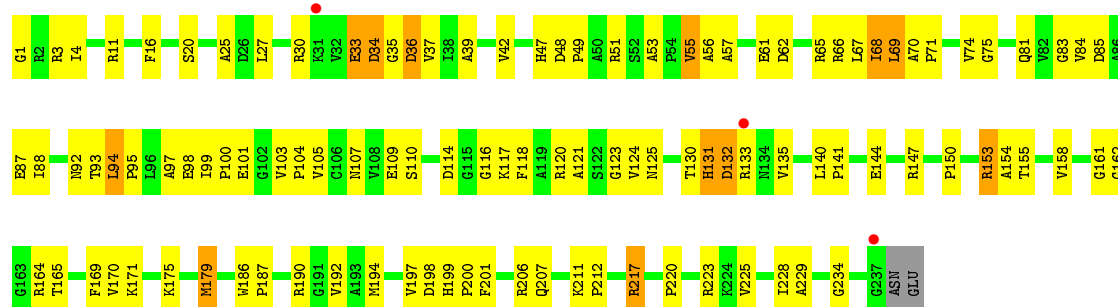
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

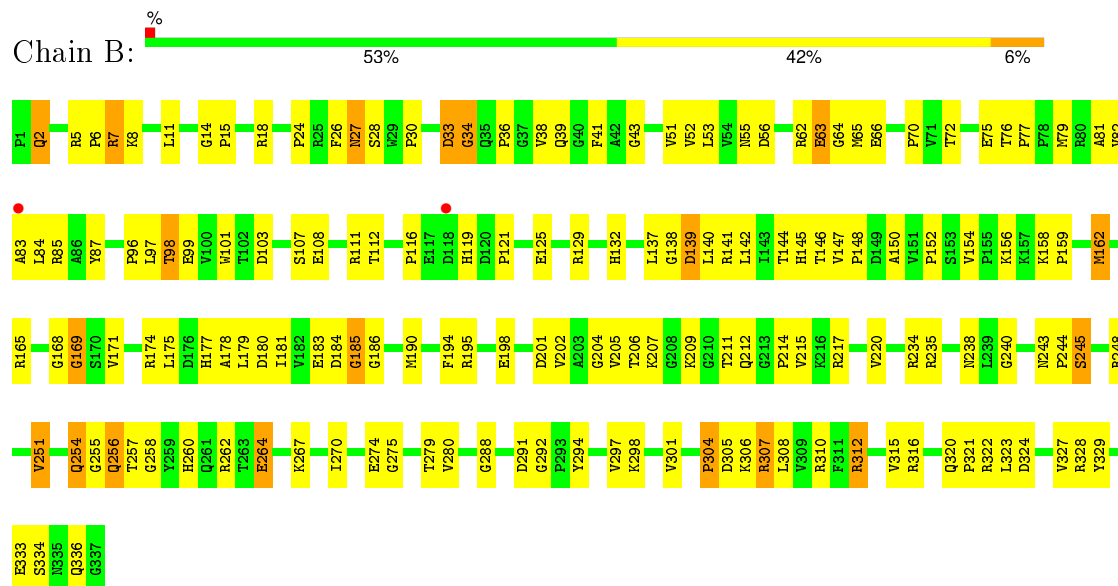
• Molecule 1: 23S RIBOSOMAL RNA



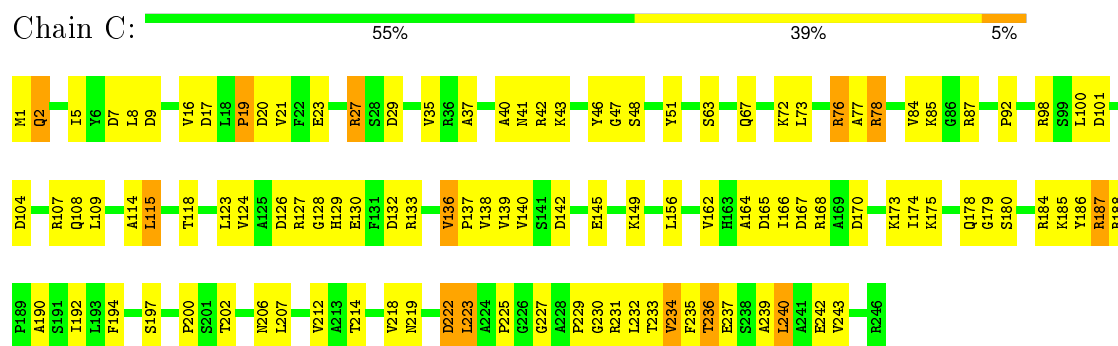




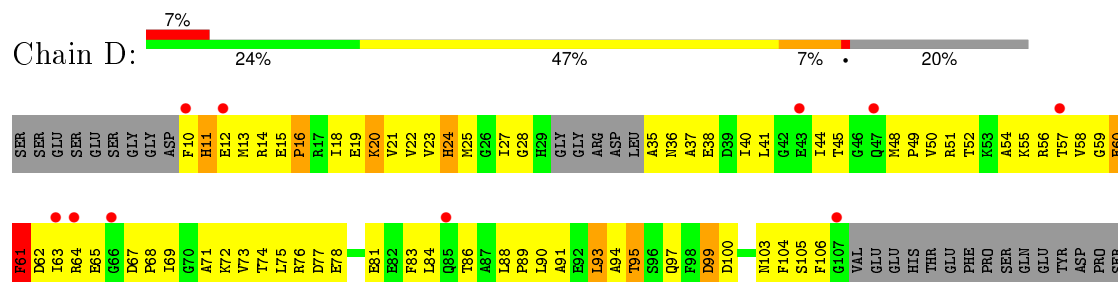
• Molecule 5: RIBOSOMAL PROTEIN L3



• Molecule 6: RIBOSOMAL PROTEIN L4

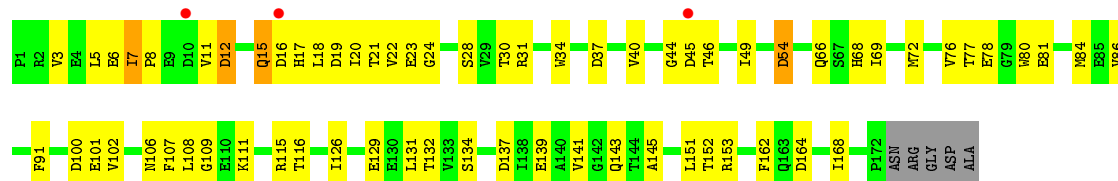


• Molecule 7: RIBOSOMAL PROTEIN L5

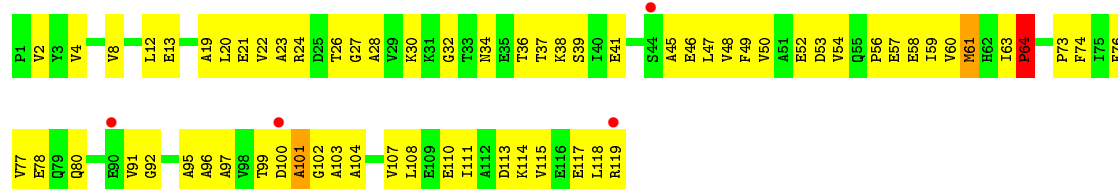
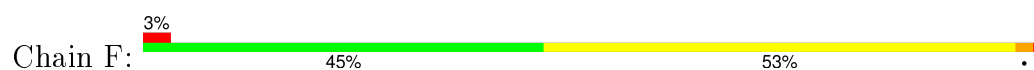




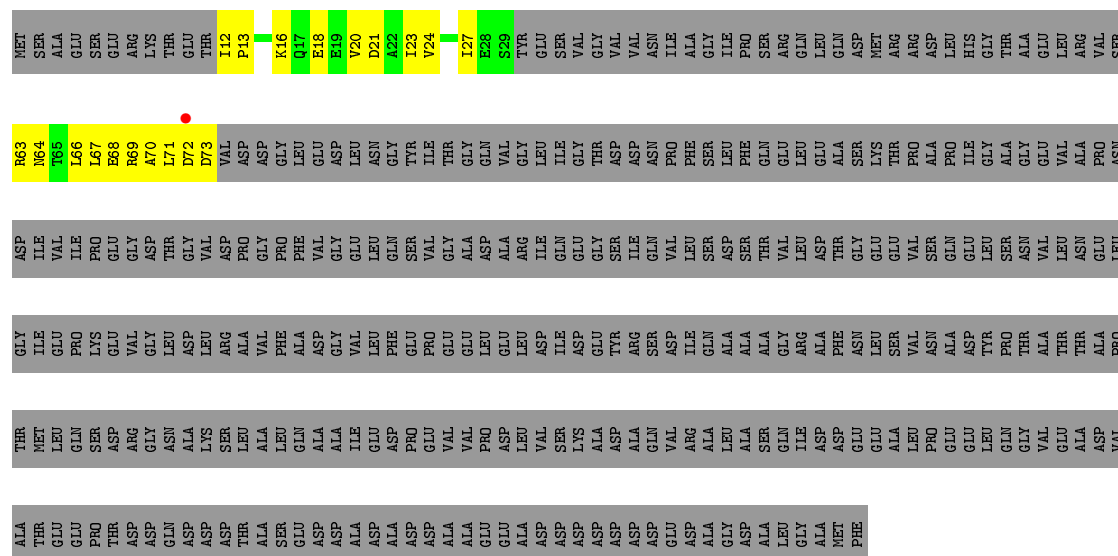
• Molecule 8: RIBOSOMAL PROTEIN L6



• Molecule 9: RIBOSOMAL PROTEIN L7AE

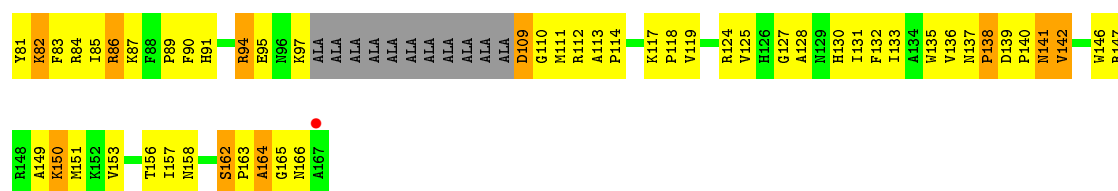


• Molecule 10: RIBOSOMAL PROTEIN L10



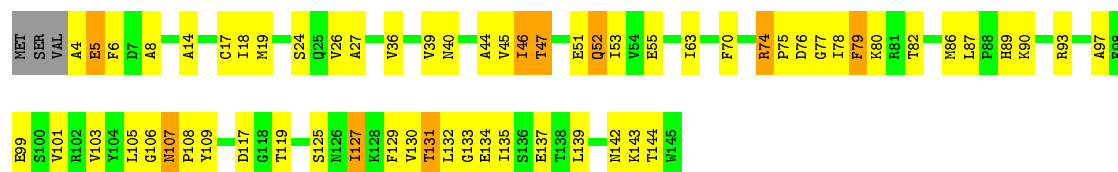
• Molecule 11: RIBOSOMAL PROTEIN L10E





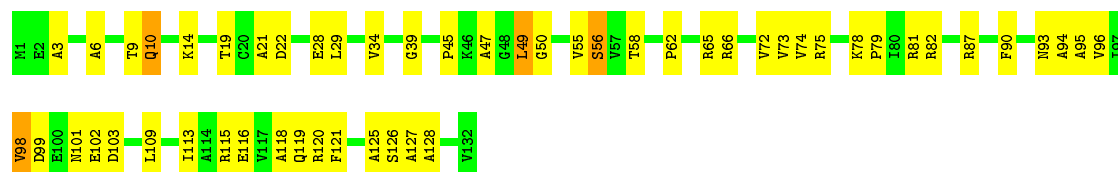
• Molecule 12: RIBOSOMAL PROTEIN L13

Chain I: 55% 37% 6%



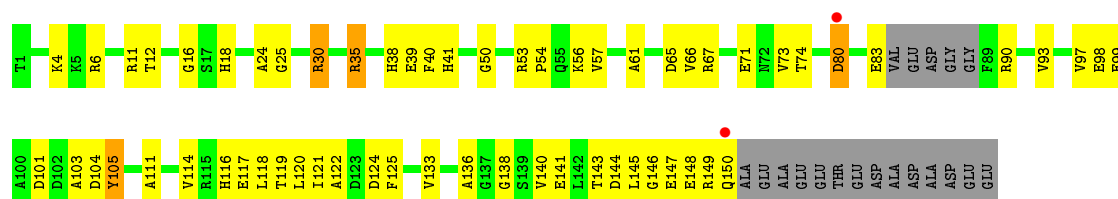
• Molecule 13: RIBOSOMAL PROTEIN L14

Chain J: 60% 37%



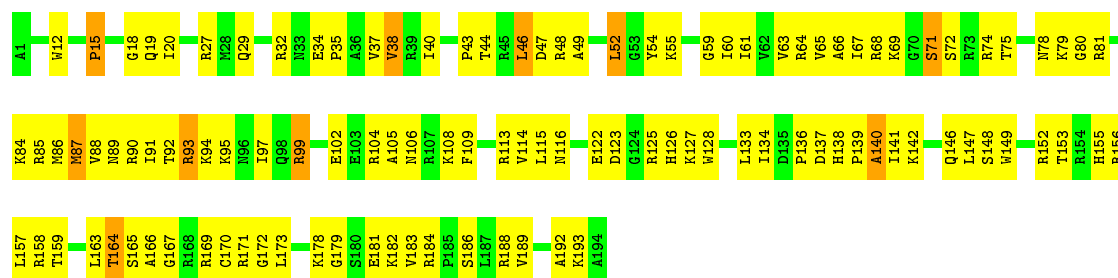
• Molecule 14: RIBOSOMAL PROTEIN L15

Chain K: 51% 35% 12%

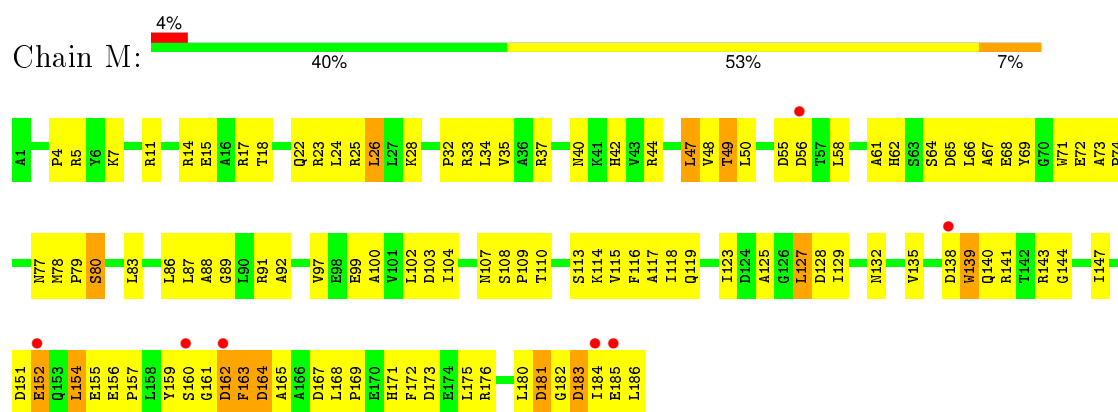


• Molecule 15: RIBOSOMAL PROTEIN L15E

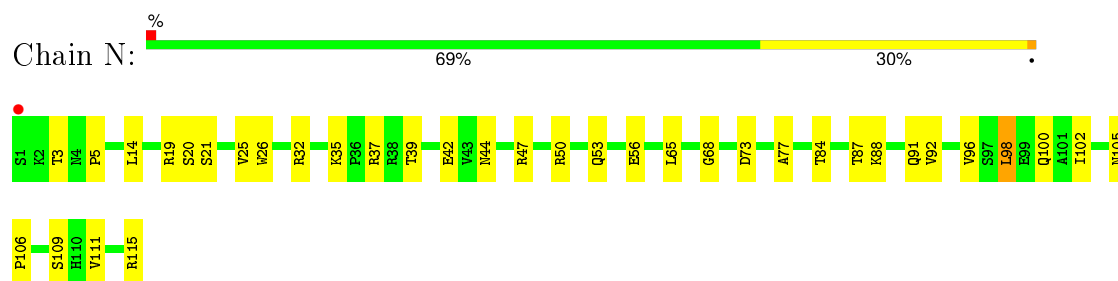
Chain L: 43% 52% 5%



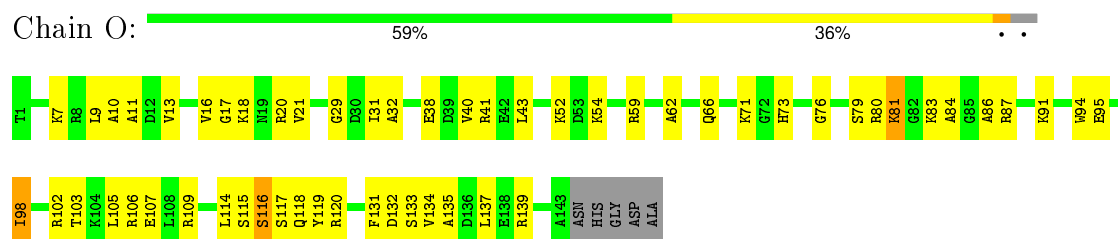
• Molecule 16: RIBOSOMAL PROTEIN L18



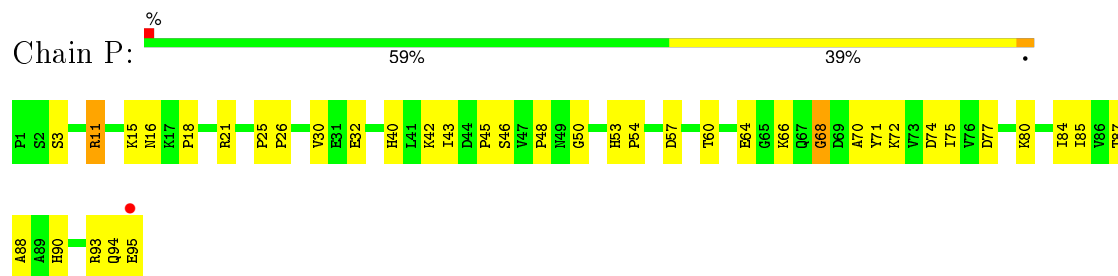
• Molecule 17: RIBOSOMAL PROTEIN L18E



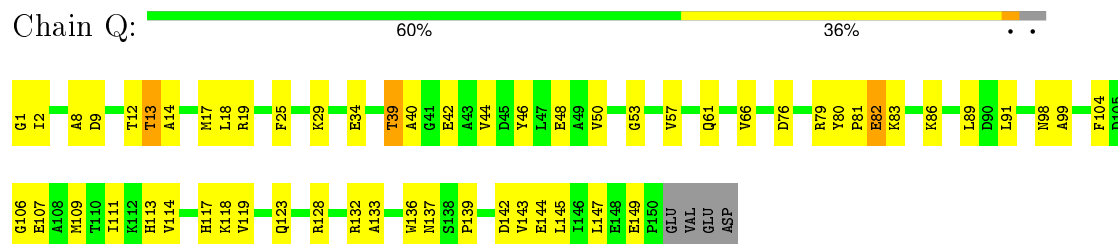
• Molecule 18: RIBOSOMAL PROTEIN L19E



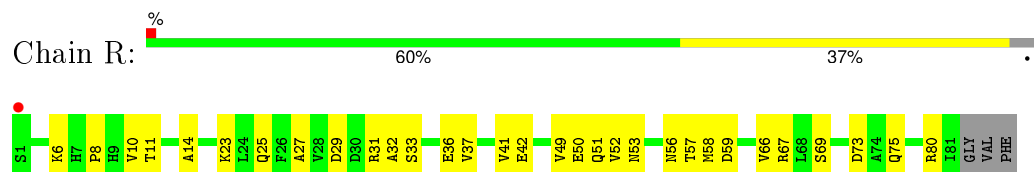
• Molecule 19: RIBOSOMAL PROTEIN L21E



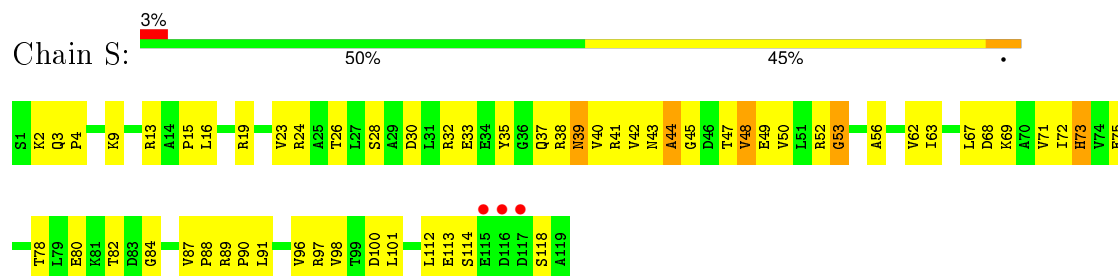
• Molecule 20: RIBOSOMAL PROTEIN L22



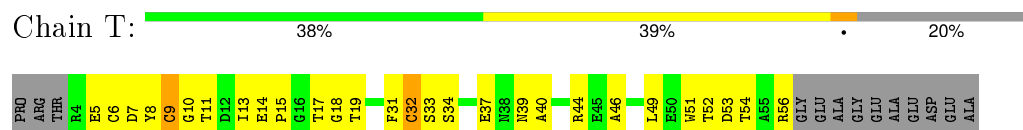
- Molecule 21: RIBOSOMAL PROTEIN L23



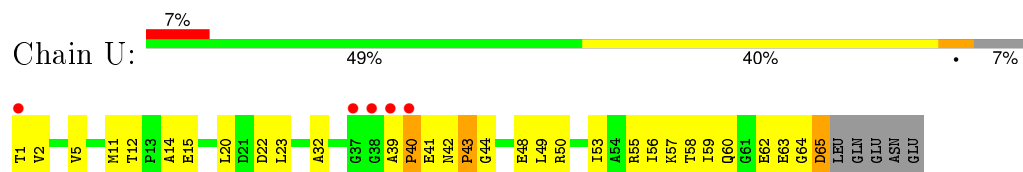
- Molecule 22: RIBOSOMAL PROTEIN L24



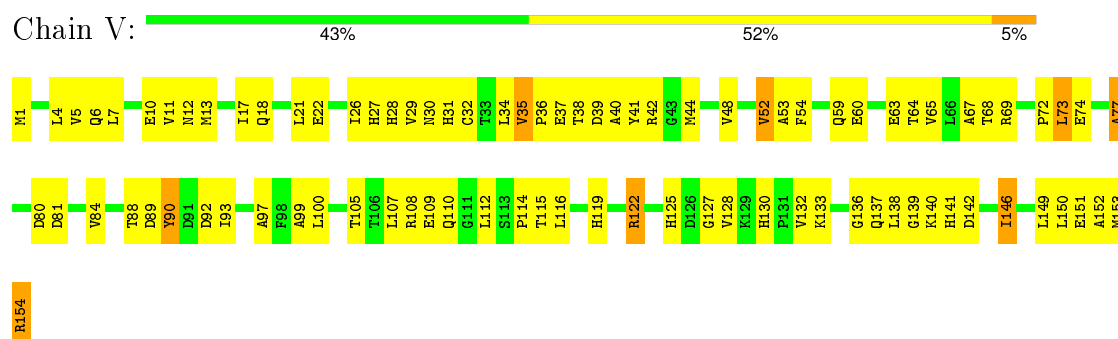
- Molecule 23: RIBOSOMAL PROTEIN L24E



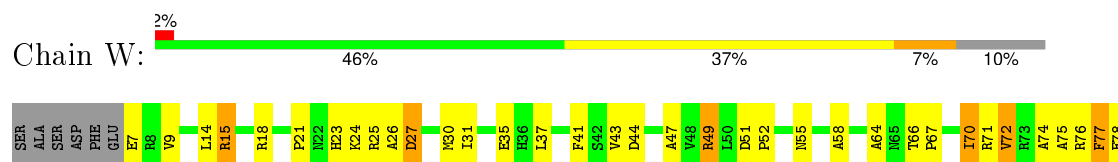
- Molecule 24: RIBOSOMAL PROTEIN L29



- Molecule 25: RIBOSOMAL PROTEIN L30



- Molecule 26: RIBOSOMAL PROTEIN L31E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.66Å 300.71Å 575.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-3.00) 90.8 (20.00-2.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.98Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.186 , 0.229 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 360129 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98635	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, SLD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.52	4/66076 (0.0%)	0.71	23/103052 (0.0%)
2	9	0.46	0/2905	0.76	3/4528 (0.1%)
3	4	0.89	0/65	1.01	0/99
4	A	0.39	0/1787	0.70	0/2409
5	B	0.40	0/2690	0.68	0/3652
6	C	0.45	0/1884	0.71	0/2551
7	D	0.37	0/1111	0.62	0/1498
8	E	0.38	0/1382	0.61	0/1880
9	F	0.38	0/897	0.60	0/1219
10	G	0.38	0/241	0.58	0/324
11	H	0.44	0/1247	0.79	3/1686 (0.2%)
12	I	0.43	0/1136	0.65	0/1530
13	J	0.41	0/1004	0.72	0/1351
14	K	0.41	0/1130	0.71	0/1509
15	L	0.49	0/1634	0.75	1/2180 (0.0%)
16	M	0.39	0/1474	0.68	0/1999
17	N	0.41	0/874	0.67	0/1181
18	O	0.41	0/1143	0.60	0/1521
19	P	0.44	0/749	0.74	1/1005 (0.1%)
20	Q	0.44	0/1172	0.69	0/1578
21	R	0.38	0/648	0.62	0/875
22	S	0.40	0/958	0.69	0/1289
23	T	0.61	2/417 (0.5%)	0.68	0/562
24	U	0.36	0/502	0.60	0/675
25	V	0.43	0/1219	0.67	0/1655
26	W	0.41	0/664	0.65	0/895
27	X	0.43	0/1146	0.68	0/1536
28	Y	0.54	1/576 (0.2%)	0.80	0/763
29	Z	0.54	0/438	0.78	2/578 (0.3%)
30	1	0.43	0/399	0.58	0/527
31	2	0.73	2/771 (0.3%)	0.72	0/1024
All	All	0.49	9/98339 (0.0%)	0.70	33/147131 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	70
2	9	0	2
25	V	0	1
All	All	0	73

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	14	CYS	CB-SG	-12.55	1.60	1.82
1	0	2102	G	C6-O6	-6.72	1.18	1.24
28	Y	60	CYS	CB-SG	-6.10	1.71	1.82
1	0	2474	A	N1-C2	5.85	1.39	1.34
23	T	9	CYS	CB-SG	-5.75	1.72	1.81

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	8.48	128.16	109.50
1	0	1979	G	C2'-C3'-O3'	6.90	124.75	113.70
11	H	74	ASN	N-CA-C	-6.85	92.50	111.00
2	9	3103	A	C5'-C4'-O4'	6.75	117.20	109.10
1	0	1563	G	C2'-C3'-O3'	6.72	124.45	113.70

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	202	U	Sidechain
1	0	223	G	Sidechain
1	0	261	A	Sidechain
1	0	324	G	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29800	1222	0
2	9	2600	0	1326	88	0
3	4	59	0	35	2	0
4	A	1754	0	1763	127	0
5	B	2625	0	2533	170	0
6	C	1859	0	1816	112	0
7	D	1094	0	1085	125	0
8	E	1357	0	1266	65	0
9	F	886	0	854	67	0
10	G	240	0	231	22	0
11	H	1216	0	1215	155	0
12	I	1120	0	1098	69	0
13	J	994	0	1027	57	0
14	K	1118	0	1076	64	0
15	L	1606	0	1676	142	0
16	M	1445	0	1401	139	0
17	N	865	0	873	35	0
18	O	1133	0	1127	57	0
19	P	735	0	729	29	0
20	Q	1149	0	1122	61	0
21	R	641	0	605	24	0
22	S	950	0	923	53	0
23	T	410	0	364	33	0
24	U	499	0	511	32	0
25	V	1196	0	1137	97	0
26	W	654	0	653	46	0
27	X	1130	0	1133	51	0
28	Y	564	0	598	54	0
29	Z	431	0	426	24	0
30	1	394	0	406	32	0
31	2	755	0	729	51	0
32	0	37	0	28	4	0
33	0	107	0	0	0	0
33	2	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	8	0	0	1	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	P	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	2	1	0	0	2	0
37	N	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5806	0	0	72	0
38	1	45	0	0	1	0
38	2	76	0	0	4	0
38	4	1	0	0	0	0
38	9	147	0	0	5	0
38	A	136	0	0	11	0
38	B	160	0	0	17	0
38	C	180	0	0	10	0
38	D	49	0	0	8	0
38	E	47	0	0	1	0
38	F	26	0	0	6	0
38	G	21	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	82	0	0	9	0
38	I	61	0	0	3	0
38	J	63	0	0	4	0
38	K	85	0	0	9	0
38	L	130	0	0	5	0
38	M	69	0	0	8	0
38	N	45	0	0	5	0
38	O	70	0	0	0	0
38	P	56	0	0	1	0
38	Q	92	0	0	4	0
38	R	40	0	0	1	0
38	S	37	0	0	3	0
38	T	27	0	0	2	0
38	U	13	0	0	1	0
38	V	74	0	0	6	0
38	W	29	0	0	3	0
38	X	105	0	0	4	0
38	Y	41	0	0	5	0
38	Z	57	0	0	1	0
All	All	98635	0	59566	2990	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 2990 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:U:12:THR:HG22	24:U:15:GLU:HG3	1.24	1.14
13:J:10:GLN:NE2	13:J:10:GLN:H	1.47	1.13
1:O:871:G:H8	1:O:871:G:H5'	1.13	1.10
11:H:86:ARG:NH1	11:H:133:ILE:HG13	1.66	1.08
15:L:87:MET:HB3	31:2:46:ILE:HD13	1.31	1.07

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	11	46
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	9	40
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	16	56
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	1	4
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	30	72
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	7	33
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	4	21
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	7	33
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	9	40
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	13	50
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	14	51
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	7	33
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	4	22
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	21	64
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	26	70
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	8	38
20	Q	148/154 (96%)	134 (90%)	14 (10%)	0	100	100
21	R	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
22	S	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11	46
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	9	41
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	27
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	26	70
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	7	34
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	3	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
30	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
31	2	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	8	38
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	9	41

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP
7	D	93	LEU
7	D	95	THR
7	D	137	PRO
7	D	173	GLU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/181 (99%)	168 (94%)	11 (6%)	23	61
5	B	282/282 (100%)	264 (94%)	18 (6%)	22	59
6	C	193/193 (100%)	178 (92%)	15 (8%)	16	49
7	D	117/147 (80%)	108 (92%)	9 (8%)	16	50
8	E	152/155 (98%)	146 (96%)	6 (4%)	39	77
9	F	92/92 (100%)	91 (99%)	1 (1%)	80	94
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	111 (91%)	11 (9%)	12	41
12	I	118/121 (98%)	110 (93%)	8 (7%)	20	56
13	J	106/106 (100%)	102 (96%)	4 (4%)	40	78
14	K	113/126 (90%)	108 (96%)	5 (4%)	35	74
15	L	166/166 (100%)	157 (95%)	9 (5%)	27	66
16	M	149/149 (100%)	141 (95%)	8 (5%)	27	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	93/93 (100%)	90 (97%)	3 (3%)	46	82
18	O	113/116 (97%)	109 (96%)	4 (4%)	43	80
19	P	79/79 (100%)	75 (95%)	4 (5%)	29	69
20	Q	117/121 (97%)	114 (97%)	3 (3%)	54	85
21	R	71/73 (97%)	69 (97%)	2 (3%)	51	84
22	S	105/105 (100%)	100 (95%)	5 (5%)	31	71
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	49 (96%)	2 (4%)	39	77
25	V	130/130 (100%)	122 (94%)	8 (6%)	23	60
26	W	66/73 (90%)	62 (94%)	4 (6%)	23	61
27	X	120/195 (62%)	113 (94%)	7 (6%)	25	63
28	Y	56/56 (100%)	52 (93%)	4 (7%)	18	54
29	Z	46/46 (100%)	45 (98%)	1 (2%)	60	88
30	1	42/44 (96%)	41 (98%)	1 (2%)	57	87
31	2	79/79 (100%)	75 (95%)	4 (5%)	29	69
All	All	3028/3441 (88%)	2871 (95%)	157 (5%)	29	68

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	I	46	ILE
14	K	117	GLU
27	X	204	ARG
12	I	52	GLN
13	J	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
14	K	41	HIS
17	N	53	GLN
30	1	16	ASN
15	L	26	HIS
16	M	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	241 (8%)	25 (0%)
2	9	121/122 (99%)	18 (14%)	3 (2%)
3	4	2/3 (66%)	1 (50%)	0
All	All	2868/3047 (94%)	260 (9%)	28 (0%)

5 of 260 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	1856	C
2	9	3024	U
1	0	1563	G
1	0	1667	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	SLD	0	9500	-	38,39,39	5.63	18 (47%)	46,53,53	2.67	19 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SLD	0	9500	-	-	0/23/51/51	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	SLD	C9S-C8S	-9.70	1.35	1.50
32	0	9500	SLD	C9S-C0S	-5.75	1.43	1.51
32	0	9500	SLD	O1-C7	-3.43	1.41	1.46
32	0	9500	SLD	C4-C2	2.07	1.43	1.39
32	0	9500	SLD	C3-C12	2.74	1.46	1.41

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	SLD	O3-C6-N1	-8.51	122.04	128.87
32	0	9500	SLD	C5-N1-C6	-5.40	108.17	111.24
32	0	9500	SLD	C9S-C0S-N5S	-3.36	109.95	117.07
32	0	9500	SLD	C7-O1-C6	-2.88	107.83	110.20
32	0	9500	SLD	O1-C6-N1	-2.77	108.18	109.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9500	SLD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.43	34 (1%) 81 55	35, 63, 107, 150	0
2	9	122/122 (100%)	0.01	5 (4%) 41 16	52, 80, 106, 150	0
3	4	3/3 (100%)	-0.41	0 100 100	49, 49, 51, 51	0
4	A	237/239 (99%)	-0.46	3 (1%) 79 53	44, 69, 101, 121	0
5	B	337/337 (100%)	-0.36	2 (0%) 90 73	42, 72, 98, 108	0
6	C	246/246 (100%)	-0.53	0 100 100	36, 63, 87, 99	0
7	D	140/176 (79%)	0.35	12 (8%) 13 4	70, 115, 131, 137	0
8	E	172/177 (97%)	-0.26	3 (1%) 73 45	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.05	4 (3%) 49 21	70, 88, 112, 118	0
10	G	29/348 (8%)	0.11	1 (3%) 49 21	85, 105, 113, 117	0
11	H	156/167 (93%)	-0.28	2 (1%) 79 53	51, 72, 100, 108	0
12	I	142/145 (97%)	-0.50	0 100 100	50, 66, 85, 102	0
13	J	132/132 (100%)	-0.37	0 100 100	53, 71, 89, 96	0
14	K	145/164 (88%)	-0.27	2 (1%) 78 51	39, 83, 117, 129	0
15	L	194/194 (100%)	-0.62	0 100 100	47, 62, 79, 90	0
16	M	186/186 (100%)	-0.02	7 (3%) 44 18	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.33	1 (0%) 85 64	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.47	0 100 100	50, 72, 87, 94	0
19	P	95/95 (100%)	-0.46	1 (1%) 82 58	51, 62, 75, 88	0
20	Q	150/154 (97%)	-0.52	0 100 100	46, 61, 81, 88	0
21	R	81/84 (96%)	-0.33	1 (1%) 81 55	59, 76, 95, 103	0
22	S	119/119 (100%)	-0.32	3 (2%) 61 30	55, 74, 97, 113	0
23	T	53/66 (80%)	-0.29	0 100 100	57, 73, 92, 99	0
24	U	65/70 (92%)	0.13	5 (7%) 16 6	68, 91, 123, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	154/154 (100%)	-0.53	0 100 100	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.23	2 (2%) 62 32	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.59	2 (1%) 78 51	43, 61, 82, 101	0
28	Y	73/73 (100%)	-0.25	0 100 100	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.70	0 100 100	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.12	2 (4%) 39 16	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.17	2 (2%) 65 35	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.37	94 (1%) 78 51	35, 69, 108, 150	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	6.3
1	0	2250	G	6.0
2	9	3025	G	4.9
22	S	116	ASP	4.9
24	U	1	THR	4.6

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8356	1/1	0.94	0.96	55.52	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8371	1/1	0.66	0.72	38.24	69,69,69,69	0
35	NA	0	8377	1/1	0.93	0.58	31.35	75,75,75,75	0
35	NA	0	8323	1/1	0.81	0.44	30.91	66,66,66,66	0
34	K	0	8202	1/1	0.81	0.77	26.95	92,92,92,92	0
35	NA	0	8378	1/1	0.84	0.77	26.66	65,65,65,65	0
35	NA	0	8376	1/1	0.95	0.46	23.49	79,79,79,79	0
35	NA	0	8372	1/1	0.93	0.74	23.45	72,72,72,72	0
36	CL	0	8505	1/1	0.83	0.43	20.77	99,99,99,99	0
35	NA	0	8303	1/1	0.94	0.50	18.70	55,55,55,55	0
33	MG	0	8064	1/1	0.94	0.36	17.82	39,39,39,39	0
35	NA	0	8321	1/1	0.94	0.41	15.67	67,67,67,67	0
35	NA	0	8368	1/1	0.77	0.36	14.46	69,69,69,69	0
35	NA	0	8361	1/1	0.72	0.37	13.98	77,77,77,77	0
36	CL	B	8519	1/1	0.88	0.38	13.66	95,95,95,95	0
35	NA	Q	8386	1/1	0.42	0.64	11.18	107,107,107,107	0
35	NA	0	8379	1/1	0.97	0.24	10.88	48,48,48,48	0
35	NA	0	8350	1/1	0.85	0.28	10.75	57,57,57,57	0
36	CL	2	8504	1/1	0.90	0.49	10.69	100,100,100,100	0
33	MG	0	8044	1/1	0.96	0.27	10.09	59,59,59,59	0
35	NA	0	8366	1/1	0.82	0.36	9.71	82,82,82,82	0
33	MG	0	8108	1/1	0.93	0.27	9.57	102,102,102,102	0
35	NA	0	8332	1/1	0.81	0.37	9.01	50,50,50,50	0
35	NA	0	8325	1/1	0.86	0.28	8.96	64,64,64,64	0
35	NA	0	8362	1/1	0.81	0.24	8.55	79,79,79,79	0
35	NA	K	8380	1/1	0.97	0.36	8.20	85,85,85,85	0
33	MG	0	8053	1/1	0.95	0.30	7.74	63,63,63,63	0
35	NA	0	8364	1/1	0.89	0.24	7.43	66,66,66,66	0
35	NA	0	8333	1/1	0.89	0.26	5.99	40,40,40,40	0
33	MG	0	8006	1/1	0.98	0.28	5.96	60,60,60,60	0
35	NA	0	8308	1/1	0.93	0.25	5.75	77,77,77,77	0
35	NA	0	8324	1/1	0.71	0.39	5.62	58,58,58,58	0
35	NA	9	8383	1/1	0.78	0.40	4.75	67,67,67,67	0
35	NA	0	8373	1/1	0.94	0.24	4.74	57,57,57,57	0
35	NA	0	8326	1/1	0.81	0.30	4.56	73,73,73,73	0
35	NA	0	8367	1/1	0.96	0.25	4.36	85,85,85,85	0
33	MG	0	8020	1/1	0.94	0.19	4.07	53,53,53,53	0
35	NA	0	8365	1/1	0.83	0.42	3.68	47,47,47,47	0
36	CL	I	8521	1/1	0.95	0.25	3.38	69,69,69,69	0
33	MG	0	8038	1/1	0.99	0.19	2.85	56,56,56,56	0
35	NA	0	8320	1/1	0.98	0.21	2.81	40,40,40,40	0
35	NA	0	8335	1/1	0.95	0.17	2.60	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8049	1/1	0.66	0.32	2.52	90,90,90,90	0
33	MG	0	8054	1/1	0.93	0.19	2.50	45,45,45,45	0
35	NA	0	8310	1/1	0.92	0.20	2.39	46,46,46,46	0
36	CL	J	8512	1/1	0.96	0.21	2.01	67,67,67,67	0
35	NA	H	8309	1/1	0.98	0.26	1.91	49,49,49,49	0
32	SLD	0	9500	37/37	0.92	0.21	1.91	46,50,53,59	0
36	CL	N	8508	1/1	0.89	0.22	1.89	116,116,116,116	0
35	NA	Q	8337	1/1	0.91	0.26	1.52	64,64,64,64	0
33	MG	0	8060	1/1	0.96	0.15	1.41	63,63,63,63	0
35	NA	0	8359	1/1	0.94	0.15	1.32	81,81,81,81	0
33	MG	0	8014	1/1	0.98	0.18	1.22	46,46,46,46	0
33	MG	0	8001	1/1	0.96	0.17	1.13	46,46,46,46	0
33	MG	0	8004	1/1	0.97	0.19	1.09	50,50,50,50	0
33	MG	0	8008	1/1	0.96	0.16	1.03	52,52,52,52	0
33	MG	0	8013	1/1	0.85	0.17	0.85	60,60,60,60	0
33	MG	X	8109	1/1	0.96	0.18	0.77	66,66,66,66	0
35	NA	0	8374	1/1	0.88	0.14	0.46	77,77,77,77	0
33	MG	0	8017	1/1	0.99	0.15	0.35	43,43,43,43	0
35	NA	0	8353	1/1	0.93	0.14	0.34	43,43,43,43	0
33	MG	0	8112	1/1	0.93	0.15	0.27	64,64,64,64	0
35	NA	0	8339	1/1	0.94	0.14	0.05	33,33,33,33	0
33	MG	A	8065	1/1	0.99	0.15	0.05	55,55,55,55	0
33	MG	0	8003	1/1	0.89	0.15	-0.04	51,51,51,51	0
33	MG	0	8077	1/1	0.98	0.13	-0.19	54,54,54,54	0
33	MG	0	8019	1/1	0.97	0.15	-0.43	43,43,43,43	0
35	NA	0	8343	1/1	0.96	0.14	-0.51	48,48,48,48	0
34	K	0	8201	1/1	0.75	0.13	-0.62	141,141,141,141	0
35	NA	0	8344	1/1	0.97	0.11	-0.64	48,48,48,48	0
35	NA	0	8331	1/1	0.98	0.12	-0.65	60,60,60,60	0
33	MG	0	8058	1/1	0.98	0.11	-0.71	61,61,61,61	0
33	MG	0	8007	1/1	0.98	0.12	-0.73	47,47,47,47	0
33	MG	0	8067	1/1	0.94	0.12	-0.73	81,81,81,81	0
35	NA	L	8347	1/1	0.96	0.13	-0.86	55,55,55,55	0
33	MG	S	8073	1/1	0.89	0.14	-0.94	71,71,71,71	0
33	MG	0	8015	1/1	0.99	0.11	-0.99	60,60,60,60	0
37	CD	Y	8403	1/1	0.98	0.07	-1.30	84,84,84,84	0
33	MG	0	8057	1/1	0.96	0.09	-1.32	53,53,53,53	0
35	NA	0	8338	1/1	0.95	0.09	-1.35	66,66,66,66	0
35	NA	0	8317	1/1	0.94	0.11	-1.38	57,57,57,57	0
33	MG	0	8086	1/1	0.97	0.06	-1.41	62,62,62,62	0
37	CD	2	8404	1/1	0.99	0.09	-1.43	90,90,90,90	0
37	CD	Z	8402	1/1	0.99	0.07	-1.50	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	I	8346	1/1	0.99	0.08	-1.52	45,45,45,45	0
33	MG	9	8052	1/1	0.96	0.10	-1.64	60,60,60,60	0
33	MG	0	8039	1/1	0.98	0.10	-1.70	53,53,53,53	0
33	MG	4	8063	1/1	0.97	0.11	-1.73	62,62,62,62	0
33	MG	0	8062	1/1	0.94	0.09	-1.77	90,90,90,90	0
33	MG	0	8074	1/1	0.98	0.07	-1.81	51,51,51,51	0
33	MG	0	8107	1/1	0.93	0.09	-1.91	55,55,55,55	0
35	NA	0	8327	1/1	0.98	0.10	-1.96	46,46,46,46	0
33	MG	0	8027	1/1	0.98	0.07	-2.00	65,65,65,65	0
33	MG	0	8010	1/1	0.99	0.10	-2.00	47,47,47,47	0
35	NA	A	8345	1/1	0.96	0.10	-2.02	48,48,48,48	0
36	CL	L	8518	1/1	0.96	0.10	-2.09	69,69,69,69	0
35	NA	P	8348	1/1	0.89	0.09	-2.14	68,68,68,68	0
33	MG	0	8002	1/1	0.97	0.09	-2.15	51,51,51,51	0
37	CD	T	8401	1/1	0.99	0.07	-2.21	83,83,83,83	0
33	MG	0	8056	1/1	0.99	0.09	-2.47	60,60,60,60	0
33	MG	0	8080	1/1	0.99	0.08	-2.66	52,52,52,52	0
33	MG	B	8055	1/1	0.95	0.06	-2.68	71,71,71,71	0
33	MG	0	8018	1/1	0.95	0.09	-2.77	57,57,57,57	0
33	MG	2	8078	1/1	0.98	0.04	-2.99	65,65,65,65	0
33	MG	0	8096	1/1	0.96	0.09	-3.15	70,70,70,70	0
33	MG	0	8016	1/1	0.96	0.07	-3.25	71,71,71,71	0
33	MG	0	8091	1/1	0.99	0.06	-3.47	65,65,65,65	0
33	MG	0	8012	1/1	0.99	0.06	-3.51	42,42,42,42	0
33	MG	0	8032	1/1	0.98	0.08	-3.70	52,52,52,52	0
35	NA	0	8305	1/1	0.97	0.08	-3.81	42,42,42,42	0
33	MG	J	8069	1/1	0.94	0.05	-3.89	87,87,87,87	0
33	MG	0	8033	1/1	0.98	0.11	-4.56	48,48,48,48	0
33	MG	0	8059	1/1	0.98	0.06	-5.88	60,60,60,60	0
33	MG	0	8084	1/1	0.99	0.05	-6.30	70,70,70,70	0
33	MG	0	8035	1/1	0.94	0.06	-6.42	69,69,69,69	0
35	NA	R	8312	1/1	0.53	0.93	-	84,84,84,84	0
33	MG	0	8099	1/1	0.93	0.23	-	80,80,80,80	0
33	MG	0	8005	1/1	0.99	0.10	-	58,58,58,58	0
33	MG	0	8093	1/1	0.98	0.10	-	63,63,63,63	0
35	NA	0	8330	1/1	0.93	0.11	-	61,61,61,61	0
33	MG	0	8104	1/1	0.92	0.13	-	66,66,66,66	0
33	MG	0	8076	1/1	0.89	0.16	-	102,102,102,102	0
35	NA	0	8316	1/1	0.84	0.21	-	52,52,52,52	0
33	MG	0	8111	1/1	0.92	0.12	-	75,75,75,75	0
35	NA	0	8340	1/1	0.78	0.36	-	69,69,69,69	0
36	CL	I	8501	1/1	0.91	0.18	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8363	1/1	0.50	0.60	-	83,83,83,83	0
33	MG	0	8045	1/1	0.89	0.25	-	91,91,91,91	0
35	NA	0	8336	1/1	0.93	0.13	-	63,63,63,63	0
33	MG	0	8022	1/1	0.88	0.57	-	83,83,83,83	0
36	CL	0	8514	1/1	0.94	0.14	-	75,75,75,75	0
33	MG	0	8041	1/1	0.98	0.24	-	68,68,68,68	0
36	CL	I	8502	1/1	0.90	0.11	-	93,93,93,93	0
33	MG	0	8026	1/1	0.96	0.08	-	39,39,39,39	0
35	NA	0	8313	1/1	0.85	0.22	-	89,89,89,89	0
36	CL	K	8510	1/1	0.83	0.26	-	104,104,104,104	0
33	MG	0	8030	1/1	0.99	0.16	-	48,48,48,48	0
35	NA	C	8304	1/1	0.93	0.38	-	51,51,51,51	0
33	MG	0	8066	1/1	0.86	0.18	-	105,105,105,105	0
33	MG	0	8029	1/1	0.95	0.07	-	60,60,60,60	0
33	MG	0	8075	1/1	0.96	0.09	-	77,77,77,77	0
36	CL	0	8515	1/1	0.86	0.29	-	100,100,100,100	0
36	CL	P	8511	1/1	0.87	0.37	-	84,84,84,84	0
33	MG	0	8114	1/1	0.78	0.70	-	95,95,95,95	0
33	MG	0	8089	1/1	0.97	0.07	-	82,82,82,82	0
33	MG	0	8115	1/1	0.93	0.12	-	73,73,73,73	0
33	MG	0	8050	1/1	0.97	0.14	-	68,68,68,68	0
36	CL	X	8520	1/1	0.97	0.28	-	57,57,57,57	0
33	MG	0	8101	1/1	0.95	0.14	-	94,94,94,94	0
33	MG	0	8098	1/1	0.98	0.06	-	50,50,50,50	0
36	CL	0	8517	1/1	0.95	0.33	-	82,82,82,82	0
35	NA	0	8375	1/1	0.91	0.69	-	81,81,81,81	0
35	NA	0	8385	1/1	0.78	0.36	-	73,73,73,73	0
33	MG	0	8048	1/1	0.98	0.06	-	66,66,66,66	0
36	CL	A	8509	1/1	0.90	0.74	-	89,89,89,89	0
33	MG	0	8094	1/1	0.99	0.07	-	97,97,97,97	0
33	MG	0	8025	1/1	0.97	0.06	-	59,59,59,59	0
33	MG	0	8116	1/1	0.94	0.16	-	84,84,84,84	0
33	MG	0	8037	1/1	0.98	0.07	-	54,54,54,54	0
35	NA	0	8329	1/1	0.56	1.25	-	98,98,98,98	0
35	NA	0	8311	1/1	0.90	0.26	-	73,73,73,73	0
35	NA	9	8351	1/1	0.33	0.26	-	94,94,94,94	0
33	MG	0	8082	1/1	0.92	0.16	-	79,79,79,79	0
33	MG	0	8042	1/1	0.96	0.14	-	61,61,61,61	0
35	NA	0	8319	1/1	0.98	0.18	-	41,41,41,41	0
36	CL	0	8522	1/1	0.97	0.64	-	92,92,92,92	0
35	NA	0	8384	1/1	0.47	0.63	-	85,85,85,85	0
33	MG	A	8105	1/1	0.82	0.30	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8031	1/1	0.96	0.12	-	54,54,54,54	0
35	NA	0	8352	1/1	0.81	0.32	-	61,61,61,61	0
33	MG	0	8061	1/1	0.99	0.05	-	45,45,45,45	0
33	MG	0	8011	1/1	0.88	0.19	-	50,50,50,50	0
35	NA	0	8370	1/1	0.90	0.40	-	76,76,76,76	0
33	MG	0	8036	1/1	0.97	0.05	-	52,52,52,52	0
35	NA	0	8328	1/1	0.88	0.23	-	55,55,55,55	0
33	MG	0	8110	1/1	0.96	0.12	-	56,56,56,56	0
36	CL	Q	8506	1/1	0.92	0.23	-	80,80,80,80	0
35	NA	0	8382	1/1	0.79	0.18	-	89,89,89,89	0
33	MG	0	8043	1/1	0.97	0.07	-	64,64,64,64	0
36	CL	0	8513	1/1	0.92	0.24	-	74,74,74,74	0
37	CD	N	8405	1/1	0.81	0.23	-	150,150,150,150	0
33	MG	0	8040	1/1	0.96	0.08	-	88,88,88,88	0
35	NA	0	8369	1/1	0.84	0.35	-	96,96,96,96	0
33	MG	0	8023	1/1	0.99	0.06	-	46,46,46,46	0
33	MG	0	8088	1/1	0.96	0.22	-	40,40,40,40	0
35	NA	0	8355	1/1	0.96	0.40	-	77,77,77,77	0
33	MG	0	8117	1/1	0.98	0.07	-	45,45,45,45	0
35	NA	0	8318	1/1	0.97	0.23	-	48,48,48,48	0
33	MG	0	8009	1/1	0.96	0.18	-	44,44,44,44	0
33	MG	0	8070	1/1	0.97	0.06	-	63,63,63,63	0
33	MG	0	8079	1/1	0.96	0.12	-	53,53,53,53	0
35	NA	0	8307	1/1	0.83	0.32	-	71,71,71,71	0
33	MG	0	8087	1/1	0.95	0.07	-	82,82,82,82	0
36	CL	0	8503	1/1	0.94	0.29	-	82,82,82,82	0
33	MG	0	8047	1/1	0.98	0.10	-	90,90,90,90	0
35	NA	0	8349	1/1	0.98	0.44	-	69,69,69,69	0
33	MG	0	8034	1/1	0.95	0.10	-	46,46,46,46	0
33	MG	0	8085	1/1	0.88	0.22	-	92,92,92,92	0
33	MG	0	8092	1/1	0.87	0.36	-	111,111,111,111	0
33	MG	0	8100	1/1	0.92	0.19	-	97,97,97,97	0
35	NA	0	8360	1/1	0.84	0.41	-	69,69,69,69	0
33	MG	0	8046	1/1	0.86	0.15	-	86,86,86,86	0
33	MG	0	8068	1/1	0.99	0.07	-	64,64,64,64	0
35	NA	0	8334	1/1	0.96	0.20	-	48,48,48,48	0
35	NA	0	8357	1/1	0.92	0.26	-	61,61,61,61	0
33	MG	0	8102	1/1	0.84	0.40	-	91,91,91,91	0
33	MG	0	8113	1/1	0.84	0.10	-	60,60,60,60	0
33	MG	0	8097	1/1	0.91	0.30	-	53,53,53,53	0
33	MG	9	8095	1/1	0.93	0.36	-	106,106,106,106	0
35	NA	0	8341	1/1	0.79	0.33	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8083	1/1	0.98	0.07	-	65,65,65,65	0
33	MG	0	8021	1/1	0.99	0.18	-	54,54,54,54	0
35	NA	0	8306	1/1	0.96	0.38	-	59,59,59,59	0
33	MG	0	8071	1/1	0.84	0.07	-	104,104,104,104	0
36	CL	M	8507	1/1	0.94	0.24	-	86,86,86,86	0
33	MG	0	8051	1/1	0.95	0.19	-	97,97,97,97	0
33	MG	0	8103	1/1	0.92	0.42	-	97,97,97,97	0
35	NA	0	8301	1/1	0.96	0.12	-	59,59,59,59	0
36	CL	0	8516	1/1	0.96	0.26	-	64,64,64,64	0
33	MG	0	8081	1/1	0.92	0.08	-	67,67,67,67	0
33	MG	0	8024	1/1	0.75	0.62	-	98,98,98,98	0
35	NA	0	8314	1/1	0.97	0.23	-	53,53,53,53	0
35	NA	0	8315	1/1	0.98	0.20	-	70,70,70,70	0
35	NA	0	8302	1/1	0.96	0.16	-	55,55,55,55	0
35	NA	0	8354	1/1	0.92	0.41	-	58,58,58,58	0
35	NA	0	8358	1/1	0.96	0.28	-	109,109,109,109	0
33	MG	0	8028	1/1	0.90	0.17	-	57,57,57,57	0
33	MG	0	8106	1/1	0.97	0.26	-	78,78,78,78	0
35	NA	0	8381	1/1	0.87	0.30	-	69,69,69,69	0
35	NA	H	8322	1/1	0.70	0.42	-	78,78,78,78	0
33	MG	0	8090	1/1	0.95	0.33	-	81,81,81,81	0
33	MG	0	8072	1/1	0.95	0.34	-	78,78,78,78	0
35	NA	0	8342	1/1	0.98	0.14	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.